

Tetrachloroethylene

127-18-4 | DTXSID2021319

Model Performance

Model

Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.91	1.08	0.91	1.08	0.92	1.00

Model Results

Predicted value: 5.25 mmHg

Global applicability domain: Inside

Local applicability domain index: 6.53e-01

Confidence level: 5.33e-01

Nearest Neighbors from the Training Set

No Similar Structures Found.